Research Proposal for PhD Programme

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PhD Thesis Title: Investigating biochemical events relevant to the small molecules and nanoscopic systems

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Biological processes in living organisms always involve biomacromolecules like proteins, DNA and RNA. However, the actual chemical event at the heart of these processes occurs within a space confined to small molecular length scales. For example, enzyme action occurs at its active site, a small region compared to the size of the entire enzyme. DNA replication and protein expression occurs over limited length scales along the nucleic acid backbone. Hence, to understand the chemical events behind a given biological process, the focus of investigation has to be within small molecular length scales.

Fluorescence activity is extremely sensitive to the immediate local environment of the fluorescent molecule, or fluorophore. [1-4]. Thus, by studying the interaction of a fluorophore with a biomacromolecule [like protein (enzymes) and DNA] responsible for a given biological reaction, it is possible to probe the physico-chemical environment of the active site of that biomacromolecule, and the response of the reaction of fluorophoric moiety towards it.

For my work, I would like to concentrate mainly on two classes of biologically relevant naturally occurring chromophoric molecules capable of emitting fluorescence: (1) Carbazole alkaloids and (2) Hydroxyflavones. Both of these two classes of natural products are ubiquitous in the plant

kingdom and abundantly found in our day-today dietary supplements. Moreover, besides being biologally active, very often they show strong fluorescence activity [5-7].

My goal is to study the interaction of these naturally occurring bioactive (antioxidant) fluorophoric compounds and their synthetic analogues with various biomacromolecules (enzyme and DNA) by spectroscopic techniques. Moreover, the electronic distribution in the fluorophoric moiety, polarity and viscosity of the medium of the study can also have immense effect on their mode of binding and nature of interaction with biomacromolecules. So it is really interesting for me to study these effects for my work.

It is also important to ascertain the potential binding sites for these compounds. For this, I would like to perform molecular dynamics and molecular modeling studies. This will also help me to find out the structural parameters of these classes of natural products and their synthetic analogues for showing their inhibitory activity and binding affinities towards biomacromolecules essential for life processes.

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